10780391s2

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LOGINID:SSPTANAG1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS 4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS 5	AUG 30	CA(SM)/CAplus(SM) Austrian patent law changes
NEWS 6	SEP 21	CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS 7	SEP 25	CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS 8	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 9	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 10	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS 11	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS 12	OCT 19	E-mail format enhanced
NEWS 13	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS 14	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 15	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 16	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 17	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS 18	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS 19	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 20	NOV 20	CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS 21	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 22	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS 23	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS 24	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS 25	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS 26	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 27	DEC 18	CA/CAplus patent kind codes updated
NEWS 28	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 29	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS 30	DEC 27	CA/CAplus enhanced with more pre-1907 records

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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 NEWS HOURS     STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN     Welcome Banner and News Items
 NEWS IPC8      For general information regarding STN implementation of IPC 8
 NEWS X25       X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that
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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:16:18 ON 05 JAN 2007

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 11:16:29 ON 05 JAN 2007
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STRUCTURE FILE UPDATES:     4 JAN 2007  HIGHEST RN 916790-89-1
DICTIONARY FILE UPDATES:    4 JAN 2007  HIGHEST RN 916790-89-1

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

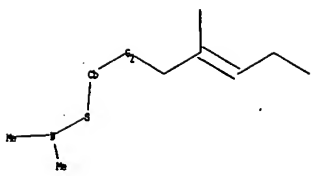
  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

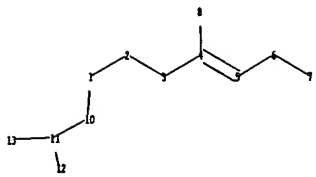
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10780391RTRs2.str
```

10780391s2





chain nodes :
1 2 3 4 5 6 7 8 10 11 12 13
chain bonds :
1-2 1-10 2-3 3-4 4-5 4-8 5-6 6-7 10-11 11-12 11-13
exact/norm bonds :
1-2 2-3 10-11
exact bonds :
1-10 3-4 4-5 4-8 5-6 6-7 11-12 11-13

G1:O,S

G2:O,S,N

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS
Element Count :
Node 1: Limited
C,C10

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR

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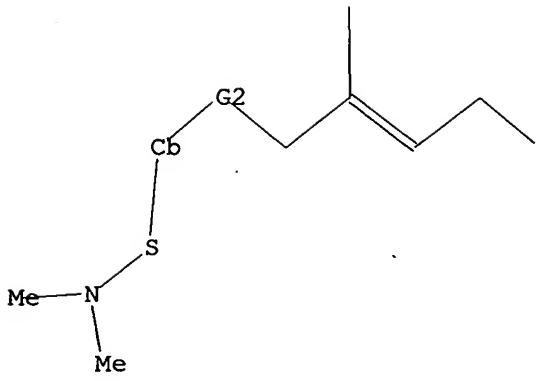

G1 O,S

G2 O,S,N

Structure attributes must be viewed using STN Express query preparation.

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=> s l1
SAMPLE SEARCH INITIATED 11:16:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       26 TO ITERATE

100.0% PROCESSED       26 ITERATIONS                                1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          215 TO      825
PROJECTED ANSWERS:               1 TO       80

L2             1 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 11:16:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      458 TO ITERATE

100.0% PROCESSED      458 ITERATIONS                               11 ANSWERS
SEARCH TIME: 00.00.01

L3            11 SEA SSS FUL L1

=> fil hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   172.10     172.31

FILE 'HCAPLUS' ENTERED AT 11:16:55 ON 05 JAN 2007
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FILE COVERS 1907 - 5 Jan 2007 VOL 146 ISS 3
FILE LAST UPDATED: 4 Jan 2007 (20070104/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3
L4 2 L3

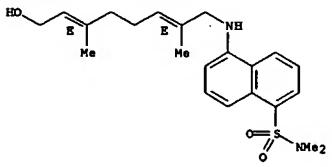
=> d ed ibib abs hitstr 1-2

L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 05 Oct 2004
ACCESSION NUMBER: 2004:807711 HCAPLUS
DOCUMENT NUMBER: 142:6669
TITLE: Synthesis and Activity of Fluorescent Isoprenoid Pyrophosphate Analogues
AUTHOR(S): Kim, MeeKyoung; Kleckley, Troy S.; Wiemer, Andrew J.; Holstein, Sarah A.; Hohl, Raymond J.; Wiemer, David F.
CORPORATE SOURCE: Departments of Chemistry Pharmacology and Internal Medicine, University of Iowa, Iowa City, IA, 52242-1294, USA
SOURCE: Journal of Organic Chemistry (2004), 69(24), 8186-8193
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:6669

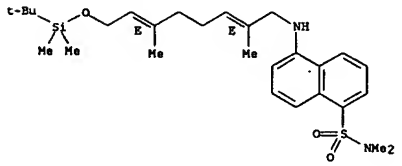
AB New fluorescent analogs of farnesol and geranylgeraniol were prepared and then converted to the corresponding pyrophosphates. These analogs incorporate anthranylate or dansyl-like groups anchored to the terpenoid skeleton through amine bonds that would be expected to be relatively stable to metabolism After addition of the alcs. or the pyrophosphates to the culture medium, their fluorescence is readily observed inside a human-derived leukemia cell line. Enzyme assays have revealed that the farnesyl pyrophosphate analog is an inhibitor of FTase, while the corresponding alc. is not. These results, together with Western blot analyses of cell lysates, indicate that the farnesyl pyrophosphate analog penetrates the cells as an intact pyrophosphate and that it does so at a biol. relevant concentration

IT 491861-22-4P
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 491861-22-4 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

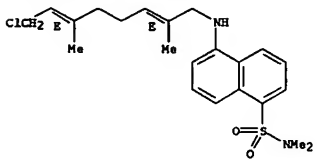


L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 798573-66-7 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-chloro-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

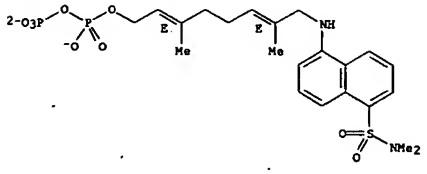


RN 798573-68-9 HCAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, (2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl (diphosphate) (3:1) (9CI) (CA INDEX NAME)

CM 1

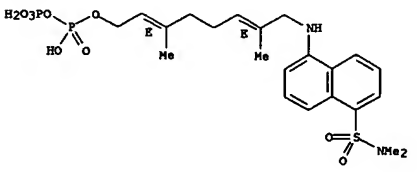
CRN 798573-67-8
CMF C22 H29 N2 O9 P2 S

Double bond geometry as shown.



L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 798573-69-0P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 798573-69-0 HCAPLUS
CN Diphosphoric acid, mono[(2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester, triammonium salt (9CI) (CA INDEX NAME)

Double bond geometry as shown.



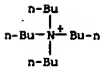
●3 NH3

IT 798573-65-6P 798573-66-7P 798573-68-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 798573-65-6 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

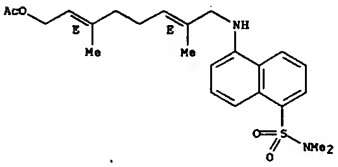
L4 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CM 2

CRN 10549-76-5
CMF C16 H36 N



IT 798573-64-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 798573-64-5 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-(acetyloxy)-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 31 Jan 2003
ACCESSION NUMBER: 2003:77548 HCAPLUS
DOCUMENT NUMBER: 138:142470
TITLE: Isoprenoid analog compounds and methods of making and use thereof
INVENTOR(S): Wiemer, David; Hohl, Raymond J.
PATENT ASSIGNEE(S): University of Iowa Research Foundation, USA
SOURCE: U.S. Pat. Appl. Publ., 18 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003022869	A1	20030130	US 2002-116737	20020403
US 6727234	B2	20040427		
US 2004167102	A1	20040826	US 2004-780391	20040217
PRIORITY APPLN. INFO.:			US 2001-281170P	P 20010403
			US 2002-116737	A3 20020403

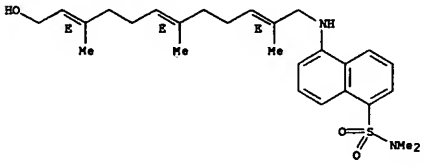
OTHER SOURCE(S): MARPAT 138:142470

AB The invention provides isoprenoid compds. and their pharmaceutically acceptable salts useful, for example, for blocking prenylation transferase enzymes, for probing or diagnosing protein prenylation processes, and for treating cancer in a mammal. A method of accessing the metabolic status of an enzyme comprises (a) contacting the enzyme with an effective amount of a mixture of a farnesol analog compound and a geraniol or geranylgeraniol analog compound, and (b) measuring the relative ratio of farnesylation to geranylgeranylation of the farnesol and the geraniol or geranylgeraniol analog compds. accomplished by the enzyme. The invention also provides pharmaceutical compns., and processes for preparing isoprenoid compds. and their intermediates.

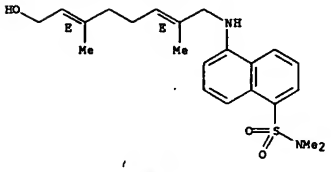
IT 491861-20-2P
RL: DGN (Diagnostic use); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(isoprenoid analog compds. for diagnosis and treatment of cancer)

RN 491861-20-2 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E,10E)-12-hydroxy-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

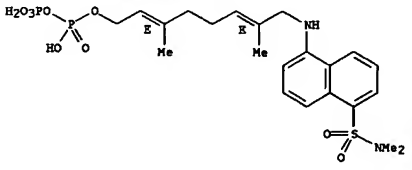


L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 491861-23-5 HCAPLUS
CN Diphosphoric acid, mono[(2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

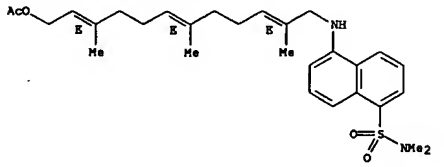


L4 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 491861-19-9P 491861-21-3P 491861-22-4P
491861-23-5P
RL: DGN (Diagnostic use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(isoprenoid analog compds. for diagnosis and treatment of cancer)

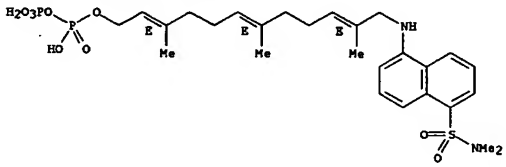
RN 491861-19-9 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E,10E)-12-(acetyloxy)-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 491861-21-3 HCAPLUS
CN Diphosphoric acid, mono[(2E,6E,10E)-12-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7,11-trimethyl-2,6,10-dodecatrienyl] ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 491861-22-4 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.14	185.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.56	-1.56

FILE 'REGISTRY' ENTERED AT 11:17:43 ON 05 JAN 2007

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 JAN 2007 HIGHEST RN 916790-89-1
DICTIONARY FILE UPDATES: 4 JAN 2007 HIGHEST RN 916790-89-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and

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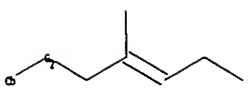
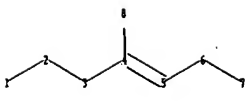
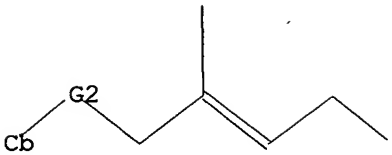




chain nodes :
1 2 3 4 5 6 7 8
chain bonds :

10780391s2



G1 O,S

G2 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 11:18:25 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 12671 TO ITERATE

15.8% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 246676 TO 260164
PROJECTED ANSWERS: 0 TO 0

10780391s2

26, 1996), unless otherwise indicated in the original publications.

FILE COVERS 1907 - 5 Jan 2007 VOL 146 ISS 3
FILE LAST UPDATED: 4 Jan 2007 (20070104/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

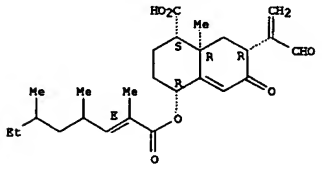
This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l7
L8 20 L7

=> d ed ibib abs hitstr 1-20

L8 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 05 Sep 2005
ACCESSION NUMBER: 2005:967021 HCAPLUS
DOCUMENT NUMBER: 144:208564
TITLE: New eremophilane-type sesquiterpenoids, eremoxylarins A and B from xylariaceous endophytic fungus YUA-026
AUTHOR(S): Shiono, Yoshihito; Murayama, Tetsuya
CORPORATE SOURCE: Department of Bioresource Engineering, Faculty of Agriculture, Yamagata University, Tsuruoka, Yamagata, 997-8555, Japan
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (2005), 60(8), 885-890
CODEN: ZNBSEN; ISSN: 0932-0776
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two new eremophilane sesquiterpenes, eremoxylarins A and B, were isolated from the xylariaceous endophytic fungus YUA-026. Their structures were determined by spectroscopic methods. Eremoxylarins A and B showed antimicrobial activity against Staphylococcus aureus and Pseudomonas aeruginosa.
IT 875760-50-2P, Eremoxylarin B
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(new eremophilane-type sesquiterpenoids eremoxylarins A and B from xylariaceous endophytic fungus YUA-026 with antimicrobial activity against Staphylococcus aureus and Pseudomonas aeruginosa)
RN 875760-50-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-4-[[(2E)-2,4,6-trimethyl-1-oxo-2-octenyl]oxy]-, (1S,4R,7R,8aR)- (9CI) (CA INDEX NAME)

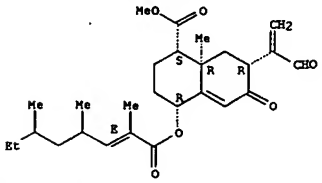
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



IT 875760-52-4P, Eremoxylarin B methyl ester
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(new eremophilane-type sesquiterpenoids eremoxylarins A and B from xylariaceous endophytic fungus YUA-026 with antimicrobial activity against Staphylococcus aureus and Pseudomonas aeruginosa)
RN 875760-52-4 HCAPLUS

L8 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1-Naphthalenecarboxylic acid, 7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-4-[[(2E)-2,4,6-trimethyl-1-oxo-2-octenyl]oxy]-, methyl ester, (1S,4R,7R,8aR)- (9CI) (CA INDEX NAME)

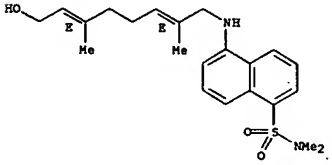
Absolute stereochemistry.
Double bond geometry as shown.
Currently available stereo shown.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 05 Oct 2004
ACCESSION NUMBER: 2004:807711 HCAPLUS
DOCUMENT NUMBER: 142:6669
TITLE: Synthesis and Activity of Fluorescent Isoprenoid Pyrophosphate Analogues
AUTHOR(S): Kim, MeeKyoung; Kleckley, Troy S.; Wiemer, Andrew J.; Holstein, Sarah A.; Hohl, Raymond J.; Wiemer, David F.
CORPORATE SOURCE: Departments of Chemistry Pharmacology and Internal Medicine, University of Iowa, Iowa City, IA, 52242-1294, USA
SOURCE: Journal of Organic Chemistry (2004), 69(24), 8186-8193
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:6669
AB New fluorescent analogs of farnesol and geranylgeraniol were prepared and then converted to the corresponding pyrophosphates. These analogs incorporate anthranylate or dansyl-like groups anchored to the terpenoid skeleton through amine bonds that would be expected to be relatively stable to metabolism After addition of the alcs. or the pyrophosphates to the
culture medium, their fluorescence is readily observed inside a human-derived
leukemia cell line. Enzyme assays have revealed that the farnesyl pyrophosphate analog is an inhibitor of FTase, while the corresponding alc. is not. These results, together with Western blot analyses of cell lysates, indicate that the farnesyl pyrophosphate analog penetrates the cells as an intact pyrophosphate and that it does so at a biol. relevant concentration
IT 491861-22-4P
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 491861-22-4 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

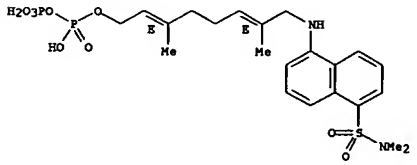
Double bond geometry as shown.



IT 798573-69-0P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of fluorescent analogs of farnesol and geranylgeraniol

L8 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 798573-69-0 HCAPLUS
CN Diphosphoric acid, mono[(2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester, triammonium salt (9CI) (CA INDEX NAME)

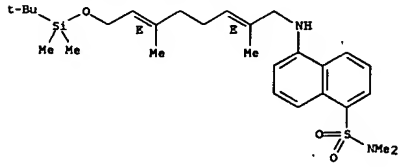
Double bond geometry as shown.



●3 NH_3

IT 798573-65-6P 798573-66-7P 798573-68-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 798573-65-6 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

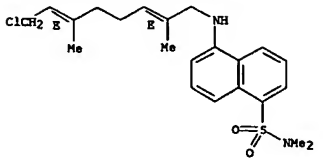
Double bond geometry as shown.



RN 798573-66-7 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-chloro-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L8 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

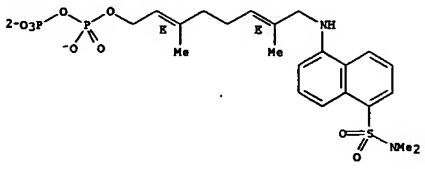


RN 798573-68-9 HCAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, (2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl (diphosphate) (3:1) (9CI) (CA INDEX NAME)

CM 1

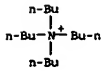
CRN 798573-67-8
CMF C22 H29 N2 O9 P2 S

Double bond geometry as shown.



CM 2

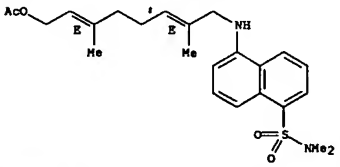
CRN 10549-76-5
CMF C16 H36 N



IT 798573-64-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl

L8 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
transferase)
RN 798573-64-5 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-(acetyloxy)-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



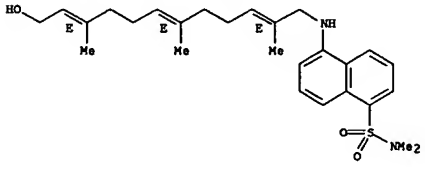
REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 31 Jan 2003
ACCESSION NUMBER: 2003:77548 HCAPLUS
DOCUMENT NUMBER: 138:142470
TITLE: Isoprenoid analog compounds and methods of making and use thereof
INVENTOR(S): Wiemer, David; Hohl, Raymond J.
PATENT ASSIGNEE(S): University of Iowa Research Foundation, USA
SOURCE: U.S. Pat. Appl. Publ., 18 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003022869	A1	20030130	US 2002-116737	20020403
US 6727234	B2	20040427		
US 2004167102	A1	20040826	US 2004-780391	20040217
PRIORITY APPLN. INFO.:			US 2001-281170P	P 20010403
			US 2002-116737	A3 20020403

OTHER SOURCE(S): MARPAT 138:142470
AB The invention provides isoprenoid compds. and their pharmaceutically acceptable salts useful, for example, for blocking prenylation transferase enzymes, for probing or diagnosing protein prenylation processes, and for treating cancer in a mammal. A method of accessing the metabolic status of an enzyme comprises (a) contacting the enzyme with an effective amount of a mixture of a farnesol analog compound and a geraniol or geranylgeraniol analog compound, and (b) measuring the relative ratio of farnesylation to geranylgeranylation of the farnesol and the geraniol or geranylgeraniol analog compds. accomplished by the enzyme. The invention also provides pharmaceutical compns., and processes for preparing isoprenoid compds. and their intermediates.
IT 491861-20-2P
RL: DGN (Diagnostic use); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(isoprenoid analog compds. for diagnosis and treatment of cancer)
RN 491861-20-2 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E,10E)-12-hydroxy-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

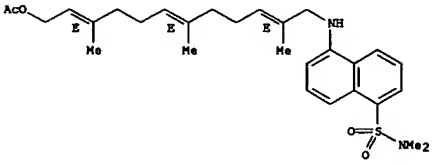
Double bond geometry as shown.



IT 491861-19-9P 491861-21-3P 491861-22-4P
491861-23-5P
RL: DGN (Diagnostic use); SPN (Synthetic preparation); THU (Therapeutic

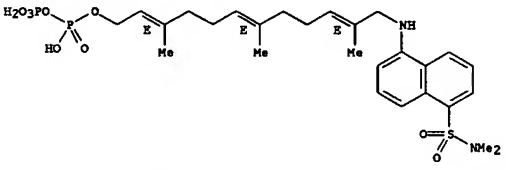
L8 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(isoprenoid analog compds. for diagnosis and treatment of cancer)
RN 491861-19-9 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E,10E)-12-(acetyloxy)-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



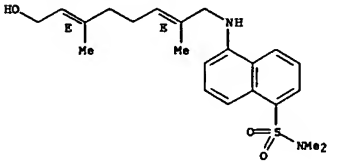
RN 491861-21-3 HCAPLUS
CN Diphosphoric acid, mono[(2E,6E,10E)-12-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7,11-trimethyl-2,6,10-dodecatrienyl] ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



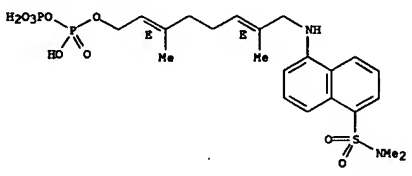
RN 491861-22-4 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L8 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 491861-23-5 HCAPLUS
CN Diphosphoric acid, mono[(2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester (9CI) (CA INDEX NAME)

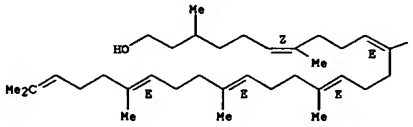
Double bond geometry as shown.



L8 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 10 Apr 2001
ACCESSION NUMBER: 2001:252486 HCAPLUS
DOCUMENT NUMBER: 135:19790
TITLE: Synthesis of dolichyl phosphates with a fluorescent label in the γ-isoprene unit of the chain
AUTHOR(S): Grigorieva, N. Ya.; Pinsker, O. A.; Mal'tsev, S. D.; Danilov, L. L.; Shibaev, V. N.; Jedrzejas, M. J.
CORPORATE SOURCE: N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, 117913, Russia
SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (2000), 49(12), 2065-2071
CODEN: RCBUEY; ISSN: 1066-5285
PUBLISHER: Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:19790
AB Stereoselective synthesis of the dolichyl phosphate derivs. WT3C2S-OP and WT2C6,7S-OP containing the 1-naphthylamino group in the γ-isoprene unit of the chain was performed. The synthetic scheme includes directed aldol condensation to construct (E)-α,β-disubstituted acroleins, their reductive amination with 1-aminonaphthalene, and phosphorylation of the resulting amino alcs.
IT 343311-91-1P 343312-11-8P 343312-12-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of dolichyl phosphates with a fluorescent label)
RN 343311-91-1 HCAPLUS
CN 6,10,14,18,22,26-Octacosahexaen-1-ol, 3,7,15,19,23,27-hexamethyl-11-[(1-naphthalenylamino)methyl]-, (6Z,10E,14E,18E,22E)- (9CI) (CA INDEX NAME)

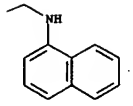
Double bond geometry as shown.

PAGE 1-A



L8 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

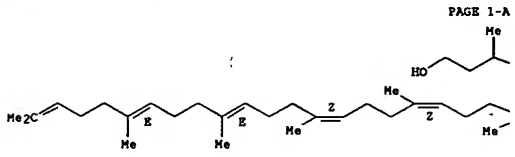
PAGE 1-B



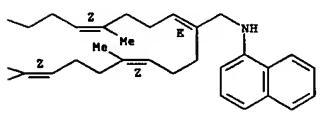
RN 343312-11-8 HCAPLUS
CN 6,10,14,18,22,26,30,34,38-Tetracontanonaen-1-ol, 3,7,15,19,23,27,31,35,39-nonamethyl-11-[(1-naphthalenylamino)methyl]-, (6Z,10E,14Z,18Z,22Z,26Z,30E,34E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

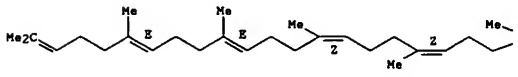


RN 343312-12-9 HCAPLUS
CN 6,10,14,18,22,26,30,34,38,42-Tetratetracontadecaen-1-ol, 3,7,15,19,23,27,31,35,39,43-decamethyl-11-[(1-naphthalenylamino)methyl]-, (6Z,10E,14Z,18Z,22Z,26Z,30Z,34E,38E)- (9CI) (CA INDEX NAME)

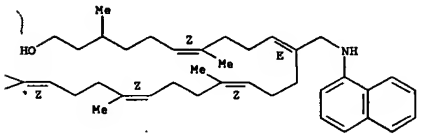
Double bond geometry as shown.

L8 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



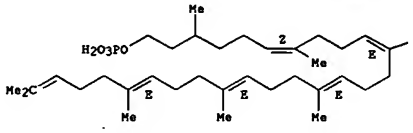
PAGE 1-B



IT 343311-92-2P 343311-99-9P 343312-00-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of dolichyl phosphates with a fluorescent label)
RN 343311-92-2 HCAPLUS
CN 6,10,14,18,22,26-Octacosahexaen-1-ol, 3,7,15,19,23,27-hexamethyl-11-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (6Z,10E,14E,18E,22E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

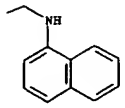
PAGE 1-A



●2 NH_3

L8 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

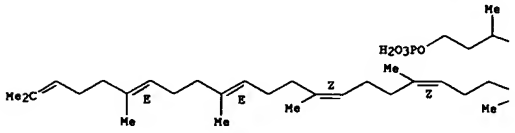
PAGE 1-B



RN 343311-99-9 HCAPLUS
CN 6,10,14,18,22,26,30,34,38-Tetracontanonaen-1-ol, 3,7,15,19,23,27,31,35,39-nonamethyl-11-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (6Z,10E,14Z,18Z,22Z,26Z,30E,34E)- (9CI) (CA INDEX NAME)

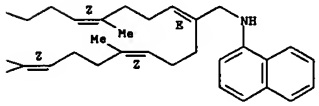
Double bond geometry as shown.

PAGE 1-A



●2 NH_3

PAGE 1-B

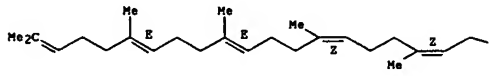


RN 343312-00-5 HCAPLUS

L8 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 6,10,14,18,22,26,30,34,38,42-Tetratetracontadecaen-1-ol, 3,7,15,19,23,27,31,35,39,43-decamethyl-11-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (6Z,10E,14Z,18Z,22Z,26Z,30Z,34E,38E)- (9CI) (CA INDEX NAME)

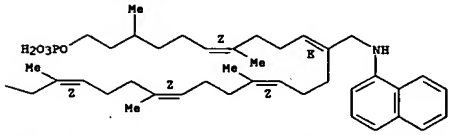
Double bond geometry as shown.

PAGE 1-A



●2 NH_3

PAGE 1-B



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

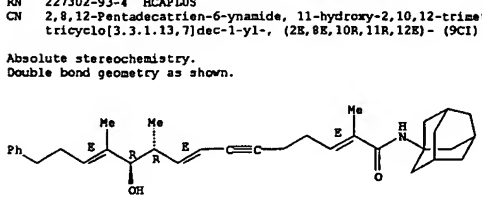
L8 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 07 Dec 2000
ACCESSION NUMBER: 2000:857079 HCAPLUS
DOCUMENT NUMBER: 134:172483
TITLE: Ultrahigh pressure liquid chromatography/time-of-flight mass spectrometry for fast separations
AUTHOR(S): Wu, Naijun; Collins, David C.; Lippert, J. Andreas; Xiang, Yanqiao; Lee, Milton L.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602-5700, USA
SOURCE: Journal of Microcolumn Separations (2000), 12(8), 462-469
CODEN: JMSEEJ; ISSN: 1040-7685
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Recently, ultraHPLC (UHPLC) was shown to overcome the pressure limitations that small particles impose on conventional pumping systems. High speed sepns. in UHPLC produce peak widths that range between 100 to 1000 ms, of which many are too narrow to be monitored by scanning mass spectrometers. The only mass spectrometer that is fast enough for such sepns. is the time-of-flight mass spectrometer (TOFMS). State-of-the-art TOFMS instruments for liquid chromatog. can record and store complete mass spectra at rates ≤100 spectra s-1. High speed sepns. with high resolution were demonstrated using 13-15 cm × 29-100 μm internal diameter capillaries packed with 1.5 μm nonporous octadecylsilane- and isohexylsilane-modified silica particles using a home-built UHPLC system. The UHPLC system was successfully coupled to TOFMS via a liquid-sheath electrospray interface. Sepns. of selected combinatorial chemical samples, pharmaceutical compds., and herbicides were completed in <100 s using UHPLC/TOFMS. Total column efficiencies ranged from 20,000-30,000 plates. The fundamental and practical aspects of UHPLC/TOFMS are discussed. Results are compared with those obtained from typical capillary LC.

IT 227302-93-4
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)
(ultrahigh pressure liquid chromatog./time-of-flight mass spectrometry for fast separation of combinatorial compds.)

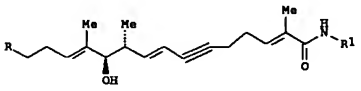
RN 227302-93-4 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-15-phenyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 20 Jul 2000
ACCESSION NUMBER: 2000:490070 HCAPLUS
DOCUMENT NUMBER: 133:266274
TITLE: The Synthesis and Evaluation of a Solution Phase Indexed Combinatorial Library of Non-Natural Polyenes for Reversal of P-Glycoprotein Mediated Multidrug Resistance
AUTHOR(S): Andrus, Merritt B.; Turner, Timothy M.; Sauna, Zuben E.; Ambudkar, Suresh V.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602-5700, USA
SOURCE: Journal of Organic Chemistry (2000), 65(16), 4973-4983
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:266274
GI



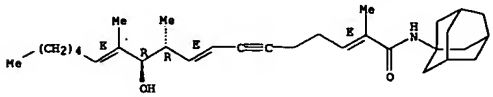
I

AB A combinatorial library of polyenes, based on (-)-stipiamide, has been constructed and evaluated for the discovery of new multidrug resistance reversal agents. A palladium coupling was used to react each individual vinyl iodide with a mixture of seven acetylenes at near 1:1 stoichiometry. The coupling was also used to react each individual acetylene with a mixture of six vinyl iodides to create 13 pools indexed in two dimensions for a total of 42 compds. Individual compds. were detected at equimolar concentration
The vinyl iodides, made initially using a crotylborane addition to generate the anti-1,2-hydroxylmethyl products, were now made using a more efficient norephedrine propionate boron enolate aldol reaction. The indexed approach, ideally suited for cellular assays that involve membrane-bound targets, allowed for the rapid identification of reversal agents using assays with drug-resistant human breast cancer MCF7-adrR cells. Intersections of potent pools identified new compds. with promising activity. Aryl dimension pools showed R = Ph and naphthyl as the most potent. The acetylene dimension had R1 = phenylalaninol and alaninol as the most potent. Isolated individual compds., both active and nonpotent, were assayed to confirm the library results. The most potent new compound was polyene I [R = 2-naphthyl, R1 = phenylalaninol] at 1.45 μM. Other nonnatural individual naphthylamide compds. showed potent MDR reversal including I [R = 2-naphthyl, R1 = morpholino] (1.69 μM). Synergistic activities attributed to the two ends of the mol. were also identified. Direct interaction with Pgp was established by ATPase and photoaffinity displacement assays. The results indicate that both ends of the polyene reversal agent are involved in Pgp interaction and can be further modified for increased potency.

IT 227302-85-4P 227302-93-4P 227303-01-7P
227303-10-8P 227303-19-7P 227303-27-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological

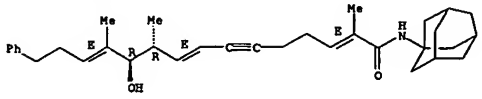
L8 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
study); PREP (Preparation)
(synthesis and evaluation of a soln. phase indexed combinatorial library of non-natural polyenes for reversal of P-glycoprotein mediated multidrug resistance)
RN 227302-85-4 HCAPLUS
CN 2,8,12-Octadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 227302-93-4 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-15-phenyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

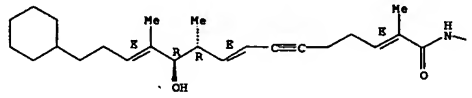
Absolute stereochemistry.
Double bond geometry as shown.



RN 227303-01-7 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 15-cyclohexyl-11-hydroxy-2,10,12-trimethyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

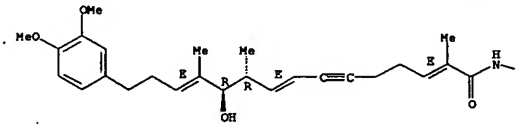
PAGE 1-A



L8 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 227303-27-7 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 15-(3,4-dimethoxyphenyl)-11-hydroxy-2,10,12-trimethyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

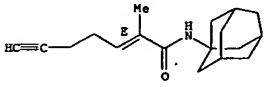
PAGE 1-A



PAGE 1-B

IT 227302-84-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and evaluation of a solution phase indexed combinatorial library of non-natural polyenes for reversal of P-glycoprotein mediated multidrug resistance)
RN 227302-84-3 HCAPLUS
CN 2-Hepten-6-ynamide, 2-methyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



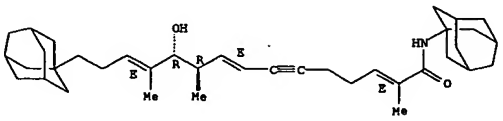
REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B

RN 227303-10-8 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-N,15-bis(tricyclo[3.3.1.13,7]dec-1-yl)-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

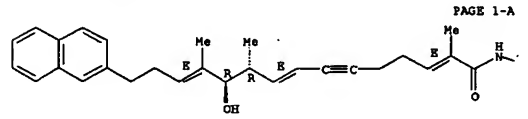
Absolute stereochemistry.
Double bond geometry as shown.



RN 227303-19-7 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-15-(2-naphthalenyl)-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

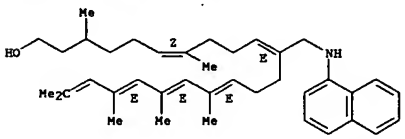
PAGE 1-A



PAGE 1-B

L8 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 19 Jun 2000
ACCESSION NUMBER: 2000:403626 HCAPLUS
DOCUMENT NUMBER: 133:252578
TITLE: Dolichyl phosphate derivatives with a fluorescent label at an internal isoprene unit
AUTHOR(S): Grigorieva, Natalia Y.; Pinsker, Ol'ga A.; Maltsev, Sergei D.; Danilov, Leonid L.; Shibaev, Vladimir N.; Jedrzejas, Mark J.
CORPORATE SOURCE: N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, 117913, Russia
SOURCE: Mendeleev Communications (2000), (3), 92-93
CODEN: MENCEX; ISSN: 0959-9436
PUBLISHER: Russian Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A general approach based on directed aldol condensation followed by reductive amination with fluorescent amines and phosphorylation was developed and illustrated by the synthesis of two dolichyl phosphate derivs. with the 1-aminonaphthalene fluorophore at the γ-isoprene unit of the chain.
IT 294846-40-5P 294846-48-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dolichyl phosphate derivs. with a fluorescent label at internal isoprene unit)
RN 294846-40-5 HCAPLUS
CN 6,10,14,16,18,20-Docosahexaen-1-ol, 3,7,15,17,19,21-hexamethyl-11-[(1-naphthalenylamino)methyl]-, (6Z,10E,14E,16E,18E)- (9CI) (CA INDEX NAME)

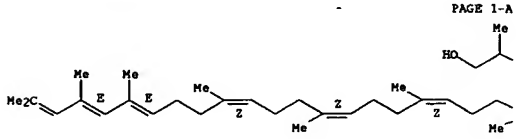
Double bond geometry as shown.



RN 294846-48-3 HCAPLUS
CN 5,9,13,17,21,25,29,33,35,37-Nonatriacontadecaen-1-ol, 2,6,14,18,22,26,30,34,36,38-decamethyl-10-[(1-naphthalenylamino)methyl]-, (5Z,9E,13Z,17Z,21Z,25Z,29Z,33E,35E)- (9CI) (CA INDEX NAME)

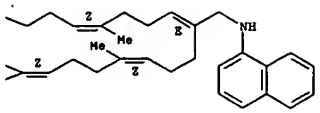
Double bond geometry as shown.

PAGE 1-A



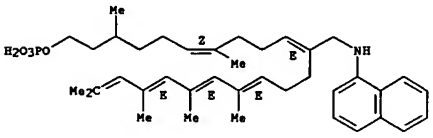
L8 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B



IT 294846-41-6P 294846-44-9P 294846-45-0P
294846-49-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of dolichyl phosphate derivs. with a fluorescent label at internal isoprene unit)
RN 294846-41-6 HCAPLUS
CN 6,10,14,16,18,20-Docosahexaen-1-ol, 3,7,15,17,19,21-hexamethyl-11-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (6Z,10E,14E,16E,18E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



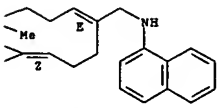
●2 NH_3

RN 294846-44-9 HCAPLUS
CN 5,9,13,17,21,25,29,31,33-Pentatriacontanonaen-1-ol, 2,6,14,18,22,26,30,32,34-nonamethyl-10-[(1-naphthalenylamino)methyl]-, (5Z,9E,13Z,17Z,21Z,25Z,29E,31E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L8 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

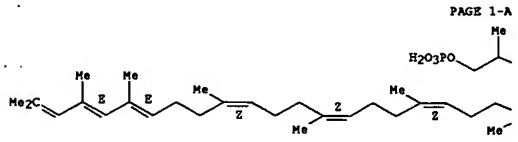
PAGE 1-B



RN 294846-49-4 HCAPLUS
CN 6,10,14,18,22,26,30,34,36,38-Tetracontadecaen-1-ol, 3,7,15,19,23,27,31,35,37,39-decamethyl-11-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (6Z,10E,14Z,18Z,22Z,26Z,30Z,34E,36E)- (9CI) (CA INDEX NAME)

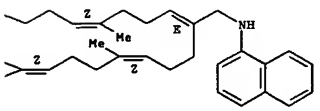
Double bond geometry as shown.

PAGE 1-A



●2 NH_3

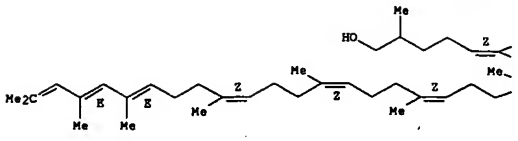
PAGE 1-B



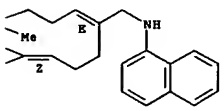
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



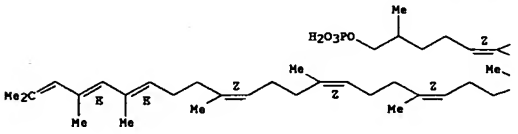
PAGE 1-B



RN 294846-45-0 HCAPLUS
CN 5,9,13,17,21,25,29,31,33-Pentatriacontanonaen-1-ol, 2,6,14,18,22,26,30,32,34-nonamethyl-10-[(1-naphthalenylamino)methyl]-, dihydrogen phosphate (ester), diammonium salt, (5Z,9E,13Z,17Z,21Z,25Z,29E,31E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

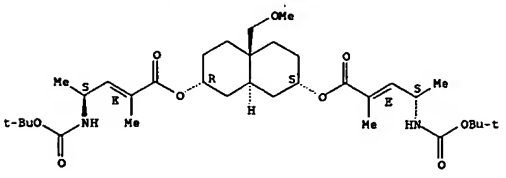
PAGE 1-A



●2 NH_3

L8 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 10 May 2000
ACCESSION NUMBER: 2000:303525 HCAPLUS
DOCUMENT NUMBER: 133:89286
TITLE: Symmetrically-substituted decalin-based scaffolds
AUTHOR(S): Plyta, Zoi F.; Heller, Eberhard; Dumas, Francoise; Miet, Christine; Mahuteau, Jacqueline; d'Angelo, Jean; Caturla, Juan; Dau, Marie-Elise Tran Huu
CORPORATE SOURCE: Centre d'Etudes Pharmaceutiques, Universite de Paris Sud, Laboratoire de Synthese Organique, BIOCIS, Unite associee au CNRS 5, Chatenay-Malabry, 92296, Fr.
SOURCE: Tetrahedron Letters (2000), 41(16), 2907-2910
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of a chiral scaffold was achieved by coupling (2R,7S)-rel-4a-[[[(1,1-dimethylethyl)phenylsilyl]oxy]methyl]decahydro-2,7-naphthalenediol with (2E,4S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-methyl-2-pentenoic acid. The target compound was (2E,4S)-4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-methyl-2-pentenoic acid (2R,7S)-4a-[[[(1,1-Dimethylethyl)phenylsilyl]oxy]methyl]decahydro-2,7-naphthalenediyl ester. The two side chains of this mol. strongly self-associate through intramol. hydrogen bonding involving the NH-BOC residues. The Mosher ester analog of the above decalin derivative was also prepared; (αR)-α-methoxy-α-(trifluoromethyl)benzeneacetic acid (2R,7S)-4a-[[[(1,1-Dimethylethyl)phenylsilyl]oxy]methyl]decahydro-2,7-naphthalenediyl ester.
IT 281193-88-2
RL: PRP (Properties)
(preparation and properties of [[(dimethylethoxy)carbonyl]amino]pentenoic acid [(silyloxy)methyl]decahydronaphthalenediyl ester)
RN 281193-88-2 HCAPLUS
CN 2-Pentenoic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-methyl-, (2α,4aβ,7α,8aα)-decahydro-4a-(methoxymethyl)-2,7-naphthalenediyl ester, (2E,2'E,4R,4'R)-rel- (9CI) (CA INDEX NAME)

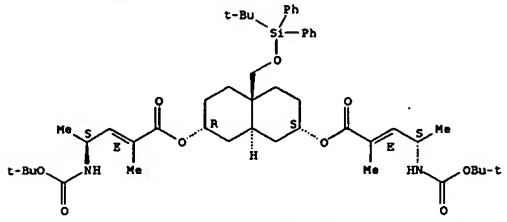
Relative stereochemistry.
Double bond geometry as shown.



IT 281193-86-0P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and properties of [[(dimethylethoxy)carbonyl]amino]pentenoic acid [(silyloxy)methyl]decahydronaphthalenediyl ester)
RN 281193-86-0 HCAPLUS
CN 2-Pentenoic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-methyl-, (2α,4aβ,7α,8aα)-4a-[[[(1,1-

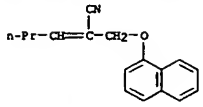
L8 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
dimethylethyl)diphenylsilyl]oxy]methyl]decahydro-2,7-naphthalenediyl ester, (2E,2'E,4R,4'R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



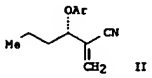
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



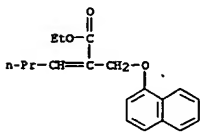
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 24 Mar 2000
ACCESSION NUMBER: 2000:188799 HCAPLUS
DOCUMENT NUMBER: 133:4276
TITLE: Deracemization of Baylis-Hillman Adducts
AUTHOR(S): Trost, Barry M.; Tsui, Hon-Chung; Toste, F. Dean
CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305-5080, USA
SOURCE: Journal of the American Chemical Society (2000), 122(14), 3534-3535
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:4276
GI



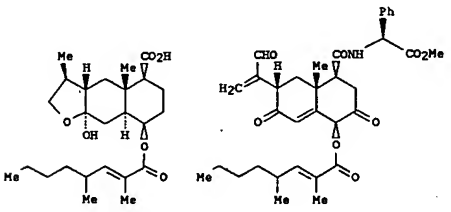
II

AB Pd2dba3 in presence of a chiral ligand catalyzed the reaction of phenols with carbonates of Baylis-Hillman adducts RCH(OCO2Me)C(EWG):CH2 (I; R = Pr, PhCH2CH2, etc.; EWG = CN, CO2Et).
IT 270903-55-4P 270903-56-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(deracemization of Baylis-Hillman adducts)
RN 270903-55-4 HCAPLUS
CN 2-Hexenoic acid, 2-[(1-naphthalenyloxy)methyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 270903-56-5 HCAPLUS
CN 2-Hexenenitrile, 2-[(1-naphthalenyloxy)methyl]- (9CI) (CA INDEX NAME)

L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 05 Mar 2000
ACCESSION NUMBER: 2000:146880 HCAPLUS
DOCUMENT NUMBER: 132:308514
TITLE: Chemical and enzymatic modifications of integric acid and HIV-1 integrase inhibitory activity
AUTHOR(S): Singh, Sheo B.; Felock, Peter; Hazuda, Daria J.
CORPORATE SOURCE: Natural Products Drug Discovery, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(3), 235-238
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

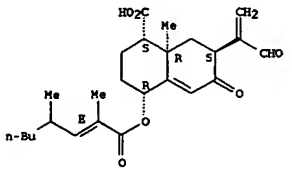


I II

AB Integric acid, an acyl eremophilane sesquiterpenoid, was identified as an inhibitor of HIV-1 integrase, the enzyme responsible for provirus entry into the host cell nucleus and integration in to the host genome. Chemical and enzymic modification of integric acid led to the preparation of several selective chemical derivs., e.g. I and II, of integric acid. Preparation, HIV-1 inhibitory activity, and the structure-activity relationship against coupled and strand transfer assays are described. It appears that most of the groups present in the natural product are required for inhibition of HIV-1 integrase strand transfer activity. In contrast, inhibition of 3' processing activity is less stringent suggesting distinct SAR for the two integrase reactions.
IT 215866-65-2, Integric acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(chemical and enzymic modifications of integric acid and HIV-1 integrase inhibitory activity)
RN 215866-65-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

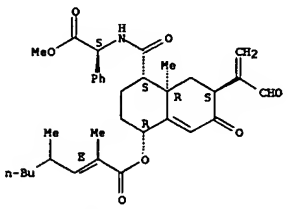
L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.
Currently available stereo shown.



IT 254976-47-1P 254976-48-2P 264255-62-1P
264255-63-2P 264255-65-4P 264255-68-7P
264255-69-8P 264255-71-2P 264255-72-3P
264255-73-4P 264255-74-5P 264255-75-6P
264255-76-7P 264255-77-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(chemical and enzymic modifications of integric acid and HIV-1 integrase inhibitory activity)

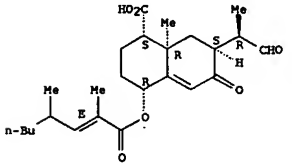
RN 254976-47-1 HCAPLUS
CN Benzeneacetic acid, α-[[[(1S,4R,7S,8aR)-4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-1-naphthalenyl]carbonyl]amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



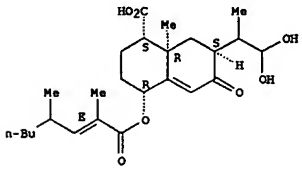
RN 254976-48-2 HCAPLUS
CN Benzeneacetic acid, α-[[[(1S,4R,7S,8aR)-4-[[(2E)-2,4-dimethyl-1-oxo-

L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



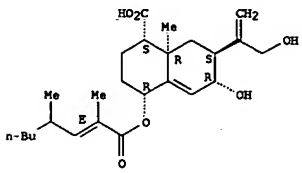
RN 264255-65-4 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 7-(2,2-dihydroxy-1-methylethyl)-4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 264255-68-7 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-6-hydroxy-7-[1-(hydroxymethyl)ethenyl]-8a-methyl-, (1S,4R,6R,7S,8aR)- (9CI) (CA INDEX NAME)

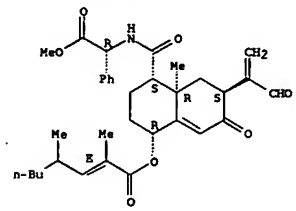
Absolute stereochemistry.
Double bond geometry as shown.



RN 264255-69-8 HCAPLUS

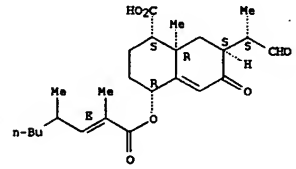
L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-1-naphthalenyl]carbonyl]amino]-, methyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.
Currently available stereo shown.



RN 264255-62-1 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-7-[(1S)-1-methyl-2-oxoethyl]-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

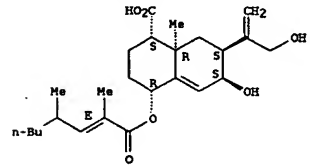


RN 264255-63-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-7-[(1R)-1-methyl-2-oxoethyl]-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

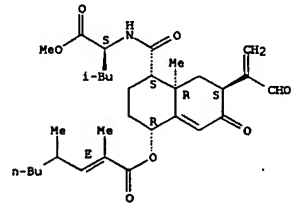
L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-6-hydroxy-7-[1-(hydroxymethyl)ethenyl]-8a-methyl-, (1S,4R,6S,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 264255-71-2 HCAPLUS
CN 2-Octenoic acid, 2,4-dimethyl-, (1R,4S,4aR,6S)-6-(1-formylethenyl)-1,2,3,4,4a,5,6,7-octahydro-4-[[[(1S)-1-(methoxycarbonyl)-3-methylbutyl]amino]carbonyl]-4a-methyl-7-oxo-1-naphthalenyl ester, (2E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

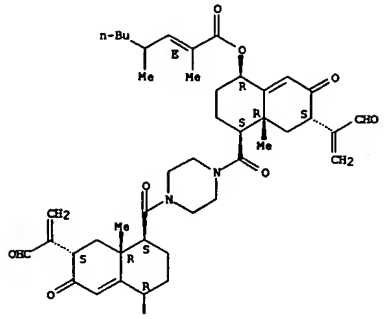


RN 264255-72-3 HCAPLUS
CN 2-Octenoic acid, 2,4-dimethyl-, 1,4-piperazinediylbis[carbonyl[(1R,4S,4aR,6S)-6-(1-formylethenyl)-1,2,3,4,4a,5,6,7-octahydro-4a-methyl-7-oxo-4,1-naphthalenediyl]] ester, (2E,2'E)- (9CI) (CA INDEX NAME)

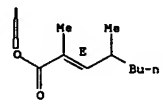
Absolute stereochemistry.
Double bond geometry as shown.

L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



PAGE 2-A

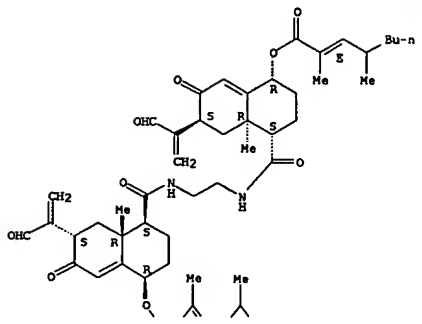


RN 264255-73-4 HCAPLUS
CN 2-Octenoic acid, 2,4-dimethyl-, 1,2-ethanediylbis[iminocarbonyl[(1R,4S,4aR,6S)-6-(1-formylethenyl)-1,2,3,4,4a,5,6,7-octahydro-4a-methyl-7-oxo-4,1-naphthalenediyl]] ester, (2E,2'E)- (9CI) (CA INDEX NAME)

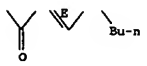
Absolute stereochemistry.
Double bond geometry as shown.

L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-A



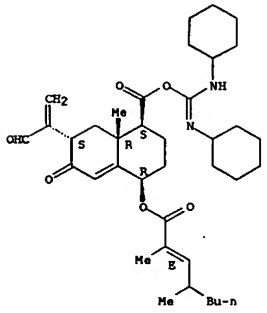
PAGE 2-A



RN 264255-74-5 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, anhydride with N,N'-dicyclohexylcarbamimidic acid, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

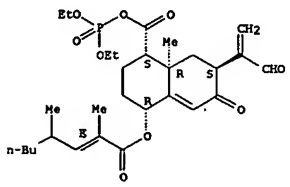
Absolute stereochemistry.
Double bond geometry as shown.

L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 264255-75-6 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, anhydride with diethyl hydrogen phosphate, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

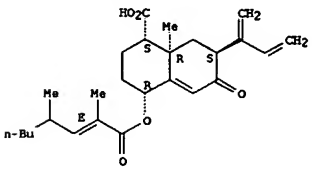
Absolute stereochemistry.
Double bond geometry as shown.



RN 264255-76-7 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-7-(1-methylene-2-propenyl)-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

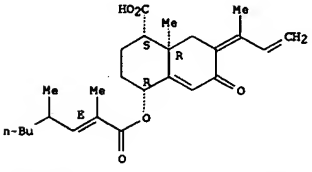
Absolute stereochemistry.
Double bond geometry as shown.

L8 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



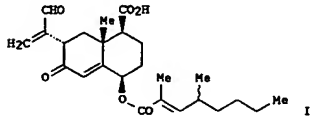
RN 264255-77-8 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-7-(1-methyl-2-propenylidene)-6-oxo-, (1S,4R,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as described by E or Z.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 09 Dec 1999
ACCESSION NUMBER: 1999:777604 HCAPLUS
DOCUMENT NUMBER: 132:90477
TITLE: Structure and absolute stereochemistry of HIV-1 integrase inhibitor integric acid. A novel eremophilane sesquiterpenoid produced by a Xylaria sp
AUTHOR(S): Singh, Sheo B.; Zink, Deborah; Polishook, Jon; Valentino, Delia; Shafiee, Ali; Silverman, Keith; Felock, Peter; Teran, Ana; Vilella, Dolores; Hazuda, Daria J.; Lingham, Russell B.
CORPORATE SOURCE: Natural Products Drug Discovery, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Tetrahedron Letters (1999), 40(50), 8775-8779
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

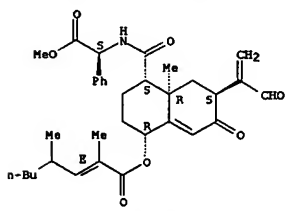
AB HIV-1 integrase is critical for viral replication and is absent in the host, and therefore is a potential target for the development of non-toxic antiviral therapy. Integric acid (I), a novel eremophilane sesquiterpenoid, was isolated from the fermentation broth of Xylaria sp. (MF6254). I inhibited 3'-end processing, strand transfer and disintegration reactions catalyzed by HIV-1 integrase with IC50 values of 3-10 μM. The isolation, structure elucidation, relative, and absolute stereochem. of integric acid were described.

IT 215866-65-2P, (+)-Integric acid
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(isolation, mol. structure, absolute configuration, and HIV-1 integrase inhibiting activity of integric acid, a novel eremophilane sesquiterpenoid metabolite of Xylaria sp. (MF6254))

RN 215866-65-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

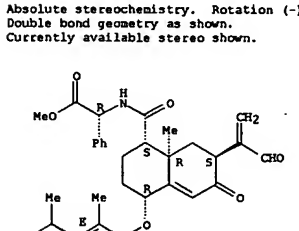
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.

L8 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



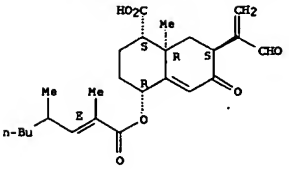
RN 254976-48-2 HCAPLUS
CN Benzeneacetic acid, α-[[[(1S,4R,7S,8aR)-4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-1-naphthalenyl]carbonyl]amino]-, methyl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.
Currently available stereo shown.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

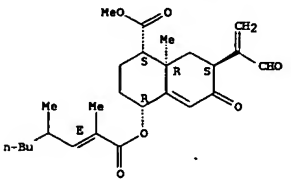
L8 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 215866-73-2P, (+)-Integric acid methyl ester 254976-47-1P 254976-48-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(isolation, mol. structure, absolute configuration, and HIV-1 integrase inhibiting activity of integric acid, a novel eremophilane sesquiterpenoid metabolite of Xylaria sp. (MF6254))

RN 215866-73-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, methyl ester, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



RN 254976-47-1 HCAPLUS
CN Benzeneacetic acid, α-[[[(1S,4R,7S,8aR)-4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-1-naphthalenyl]carbonyl]amino]-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.

L8 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Apr 1999
ACCESSION NUMBER: 1999:246151 HCAPLUS
DOCUMENT NUMBER: 131:70216
TITLE: Isolation and characterization of novel human immunodeficiency virus integrase inhibitors from fungal metabolites
AUTHOR(S): Hazuda, Daria; Blau, Carol Uncapher; Felock, Peter; Hastings, Jeffrey; Pramanik, Bernali; Wolfe, Abigail; Bushman, Frederic; Farnet, Chris; Goetz, Michael; Williams, Marie; Silverman, Keith; Lingham, Russell; Singh, Sheo
CORPORATE SOURCE: Department of Antiviral Research, Merck Research Laboratories, West Point, PA, 19486, USA
SOURCE: Antiviral Chemistry & Chemotherapy (1999), 10(2), 63-70
CODEN: ACCHEH; ISSN: 0956-3202
PUBLISHER: International Medical Press
DOCUMENT TYPE: Journal
LANGUAGE: English

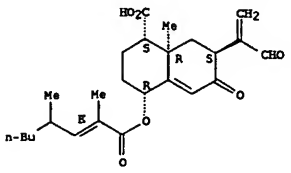
AB We have identified a series of novel inhibitors of human immunodeficiency virus type 1 (HIV-1) integrase by randomly screening natural product exts. using an in vitro biochem. assay designed to identify inhibitors of integrase-catalyzed strand transfer. Equisetin recovered from the fungus Fusarium heterosporum and a novel enantiomeric homolog of equisetin from Phoma sp. were isolated as inhibitors of HIV-1 integrase in vitro. Two addnl. analogs, a novel decalin derivative, integric acid, and oteromycin were also discovered to be inhibitors of integrase. Equisetin and related compds. inhibit 3' end-processing and strand transfer as well as disintegration catalyzed by either the full-length enzyme or the truncated integrase core domain (amino acids 50-212). These compds. also inhibit strand transfer reactions catalyzed by stable complexes assembled in vitro and integration reactions catalyzed by pre-integration complexes isolated from HIV-1-infected cells. The compds. described in this report are structurally novel and mechanistically distinct from many previously described inhibitors of HIV-1 integrase. These results demonstrate the utility of using an appropriately configured assay to identify compds. that are effective post-assembly and the potential of isolating novel integrase inhibitors from complex natural product exts.

IT 215866-65-2P, Integric acid
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(isolation and characterization of novel human immunodeficiency virus integrase inhibitors from fungal metabolites)

RN 215866-65-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.

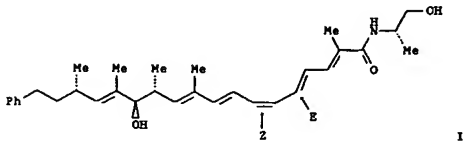
L8 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN

ED Entered STN: 16 Apr 1999
ACCESSION NUMBER: 1999:234630 HCAPLUS
DOCUMENT NUMBER: 131:44674
TITLE: The Synthesis and Evaluation of a Solution-Phase Indexed Combinatorial Library of Non-natural Polyenes for Multidrug Resistance Reversal
AUTHOR(S): Andrus, Merritt B.; Turner, Timothy M.; Asgari, Davoud; Li, Wenke
CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brigham Young University, Provo, UT, 84602-5700, USA
SOURCE: Journal of Organic Chemistry (1999), 64(9), 2978-2979 CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

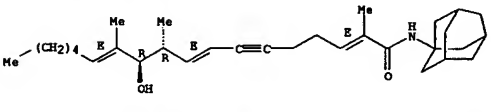
AB A solution-phase library, based on the multidrug resistance reversing polyene, (-)-stipiamide (I), that consists of mixts. indexed in two dimensions that provides for efficient combinatorial synthesis, direct screening with a cellular assay, and the isolation and testing of individual compds. is reported.

IT 227302-85-4P 227302-93-4P 227303-01-7P
227303-10-8P 227303-19-7P 227303-27-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and evaluation of a solution-phase combinatorial library of non-natural polyenes for multidrug resistance reversal)

RN 227302-85-4 HCAPLUS
CN 2,8,12-Octadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

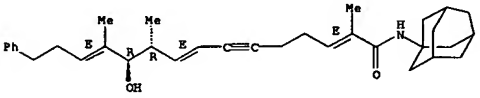
Absolute stereochemistry.
Double bond geometry as shown.

L8 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 227302-93-4 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-15-phenyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

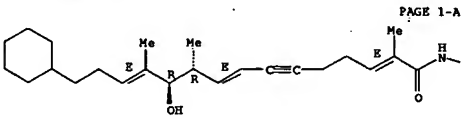
Absolute stereochemistry.
Double bond geometry as shown.



RN 227303-01-7 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 15-cyclohexyl-11-hydroxy-2,10,12-trimethyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A

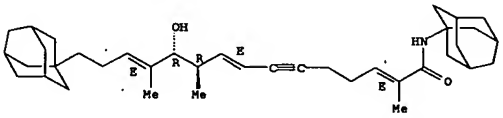


PAGE 1-B

RN 227303-10-8 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-N,15-bis(tricyclo[3.3.1.13,7]dec-1-yl)-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

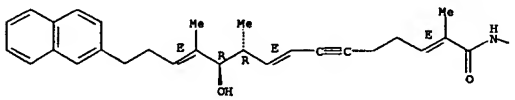
L8 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



RN 227303-19-7 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 11-hydroxy-2,10,12-trimethyl-15-(2-naphthalenyl)-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A

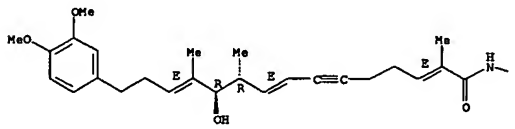


PAGE 1-B

RN 227303-27-7 HCAPLUS
CN 2,8,12-Pentadecatrien-6-ynamide, 15-(3,4-dimethoxyphenyl)-11-hydroxy-2,10,12-trimethyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E,8E,10R,11R,12E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A

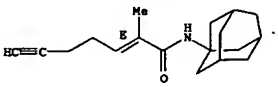


L8 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

PAGE 1-B

IT 227302-84-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and evaluation of a solution-phase combinatorial library of non-natural polyenes for multidrug resistance reversal)
RN 227302-84-3 HCAPLUS
CN 2-Hepten-6-ynamide, 2-methyl-N-tricyclo[3.3.1.13,7]dec-1-yl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 22 Jan 1999
ACCESSION NUMBER: 1999:45072 HCAPLUS
DOCUMENT NUMBER: 130:119582
TITLE: Ermophilane sesquiterpenoids as HIV integrase inhibitors
INVENTOR(S): Lingham, Russell B.; Polishook, Jon David; Shafiee, Ali; Silverman, Keith C.; Singh, Sheo Bux; Zink, Deborah L.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5858738	A	19990112	US 1997-964081	19971104

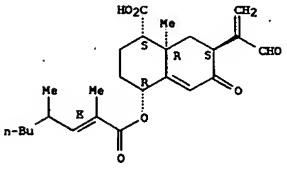
PRIORITY APPLN. INFO.: US 1997-964081 19971104
OTHER SOURCE(S): MARPAT 130:119582

AB Natural products such as certain ermophilane sesquiterpenoids and derivs. thereof are described. These compds. are useful in the inhibition of HIV integrase, the prevention or treatment of infection by HIV and the treatment of AIDS, either as compds., pharmaceutically acceptable salts, pharmaceutical composition ingredients, whether or not in combination with other antivirals, immunomodulators, antibiotics or vaccines. Methods of treating AIDS and methods of preventing or treating infection by HIV are also described. The fungal culture MF6254, Xylaria sp. (ATCC 74397) is also described and disclosed.

IT 215866-65-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(ermophilane sesquiterpenoids as HIV integrase inhibitors)
RN 215866-65-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

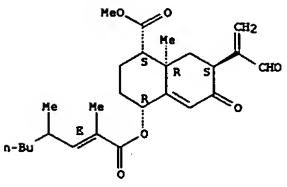
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.

L8 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 215866-73-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(ermophilane sesquiterpenoids as HIV integrase inhibitors)
RN 215866-73-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, methyl ester, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

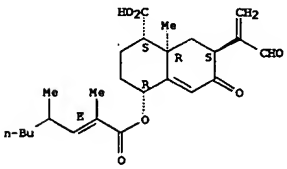
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



IT 215866-65-2D, esters
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ermophilane sesquiterpenoids as HIV integrase inhibitors)
RN 215866-65-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.

L8 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

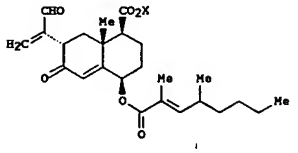


REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 18 Dec 1998
ACCESSION NUMBER: 1998:791573 HCAPLUS
DOCUMENT NUMBER: 130:10607
TITLE: HIV integrase inhibitors from culture of Xylaria species
INVENTOR(S): Lingham, Russell B.; Polishook, Jon D.; Shafiee, Ali; Silverman, Keith C.; Singh, Sheo B.; Zink, Deborah L.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Brit. UK Pat. Appl., 35 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
GB 2319026	A	19980513	GB 1997-22761		19971028
PRIORITY APPLN. INFO.:			GB 1997-22761	A	19971028
			GB 1996-25326	P	19961205
			US 1996-29886P		19961107

OTHER SOURCE(S): MARPAT 130:10607
GI



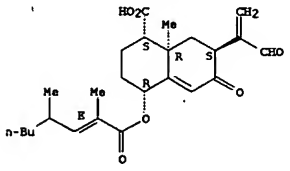
I

AB Natural products such as certain ermophilane sesquiterpenoids and derivs., useful in the inhibition of HIV integrase, the prevention or treatment of infection by HIV and the treatment of AIDS, ether as compds., pharmaceutically acceptable salts, pharmaceutical composition ingredients, whether or not in combination with other antivirals, immunomodulators, antibiotics, or vaccines are described. The compds. (I; X = H, (substituted) C1-14 alkyl) are isolated from a novel fungal culture MF6254, Xylaria sp. (ATCC 74397).

IT 215866-65-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(HIV integrase inhibitors from culture of Xylaria species)
RN 215866-65-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

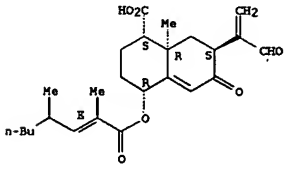
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



● K

RN 215866-69-6 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, calcium salt, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



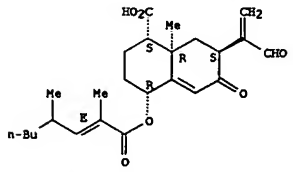
●1/2 Ca

RN 215866-70-9 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[(2,4-dimethyl-1-oxo-2-octenyl)oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1R,4S,7R,8aS)-rel-, compd. with 1,2-ethanediamine (1:1) (9CI) (CA INDEX NAME)

CM 1

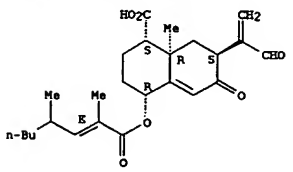
CRN 215866-65-2
CMF C25 H34 O6

L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



IT 215866-66-3P 215866-67-4P 215866-69-6P
215866-70-9P 215866-71-0P 215866-72-1P
215866-73-2P 215866-74-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(HIV integrase inhibitors from culture of Xylaria species)
RN 215866-66-3 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, ammonium salt, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.

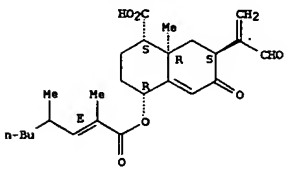


● NH_3

RN 215866-67-4 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, potassium salt, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



CM 2

CRN 107-15-3
CMF C2 H8 N2

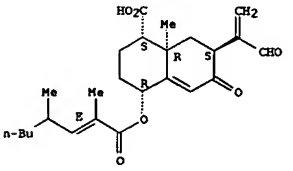
$H_2N-CH_2-CH_2-NH_2$

RN 215866-71-0 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[(2,4-dimethyl-1-oxo-2-octenyl)oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, (1R,4S,7R,8aS)-rel-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 215866-65-2
CMF C25 H34 O6

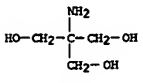
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



CM 2

L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 77-86-1
CMF C4 H11 N O3

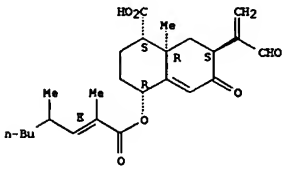


RN 215866-72-1 HCAPLUS
CN L-Lysine, mono[rel-(1R,4S,7R,8aS)-4-[(2,4-dimethyl-1-oxo-2-octenyl)oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-1-naphthalenecarboxylate] (9CI) (CA INDEX NAME)

CM 1

CRN 215866-65-2
CMF C25 H34 O6

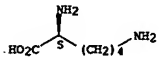
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



CM 2

CRN 56-87-1
CMF C6 H14 N2 O2

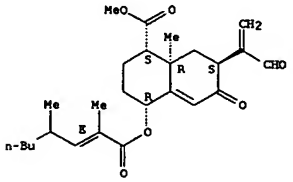
Absolute stereochemistry.



RN 215866-73-2 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[[(2E)-2,4-dimethyl-1-oxo-2-octenyl]oxy]-7-

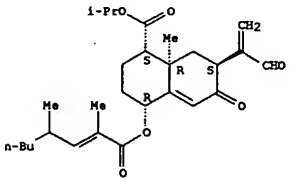
L8 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, methyl ester, (1S,4R,7S,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.
Currently available stereo shown.



RN 215866-74-3 HCAPLUS
CN 1-Naphthalenecarboxylic acid, 4-[(2,4-dimethyl-1-oxo-2-octenyl)oxy]-7-(1-formylethenyl)-1,2,3,4,6,7,8,8a-octahydro-8a-methyl-6-oxo-, 1-methylethyl ester, (1R,4S,7R,8aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

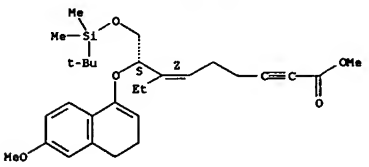


L8 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 28 May 1994
ACCESSION NUMBER: 1994:270951 HCAPLUS
DOCUMENT NUMBER: 120:270951
TITLE: Total synthesis of (+)-13-ethyl-3-methoxygona-1,3,5,9(11)-tetran-17-one via the tandem Claisen-ene strategy
AUTHOR(S): Groen-Piotrowska, E. M.; Groen, M. B.
CORPORATE SOURCE: Organon Sci. Dev. Group, Oss, 5340 BH, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1993), 112(12), 627-34
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:270951
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB A total synthesis of the title compound I, a potential precursor of the progestagens desogestrel and 3-ketodesogestrel, is described. The backbone of the steroid was assembled by condensation of 1,2-dihydronaphthalene II with 6-nonen-2-ynoic acid III (TBDMS = tert-butyldimethylsilyl) and subsequent Claisen rearrangement of the resulting enol ether to give disecosteroid IV. Heating of IV at 170° gave a 1:1 mixture of 9,11-secosteroids V and its 13α epimer. The 13β-epimer V was converted into 9,11-secogona-1,3,5(10)-triene-9,17-dione VI (X = Br), which was treated with triphenylphosphine under high pressure conditions (12 kbar, 55°) to give the corresponding phosphonium salt VI (X = P+Ph3 Br-) (VII). The intramol. Wittig reaction of VII proceeded with epimerization at C-8 to give exclusively the 8α epimer of I, which underwent isomerization upon treatment with acid to the title compound I.
IT 154619-36-0P
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(formation and Claisen rearrangement of)
RN 154619-36-0 HCAPLUS
CN 6-Nonen-2-ynoic acid, 8-[(3,4-dihydro-6-methoxy-1-naphthalenyl)oxy]-9-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-ethyl-, methyl ester, (S-(Z))- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

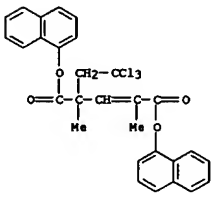


L8 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

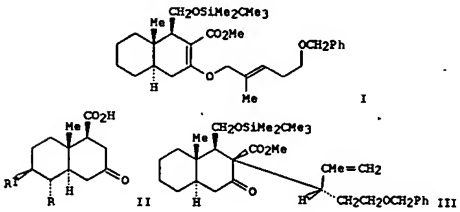
L8 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 21 Mar 1987
ACCESSION NUMBER: 1987:85169 HCAPLUS
DOCUMENT NUMBER: 106:85169
TITLE: Study on radical telomerization of esters of methacrylic acid by using bromotrichloromethane and characteristics of the resulting telomers. III. Aryl methacrylates
AUTHOR(S): Kimura, Takao; Nakanishi, Itaru; Hamashima, Motome
CORPORATE SOURCE: Fac. Eng., Utsunomiya Univ., Utsunomiya, 321, Japan
SOURCE: Polymer Journal (Tokyo, Japan) (1986), 18(10), 689-97
CODEN: POLJB8; ISSN: 0032-3896
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Radical telomerization of Ph (I), 1-naphthyl (II) and 2-naphthyl methacrylate (III) with BrCCl3 as a telogen at 50, 70, and 90° gave similar product distributions and tacticity as those of Me methacrylate (IV), but without formation of lactones. The order of the apparent rate of telomerization was IV .simeq. I > II >> III. The n[Monomer]:[BrCCl3] adducts, i.e., the n-mers (n = 1-3), were separated by silica gel column chromatog. The aryl methacrylate and IV telomers differed remarkably from each other in reactivity. The elimination reaction of the aromatic telomers with Et3N was labile and complicated in comparison with that of the IV telomers, and the dimers underwent main chain scission in addition to the normal elimination reaction. The catalytic lactonization of the aromatic dimers gave unsatd. compds. in preference to lactones, which were exclusively obtained in the pyrolysis of the IV dimers. Furthermore, the pyrolysis of the naphthyl methacrylate dimers resulted in the diastereoisomerization through depolymn.

IT 106749-91-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 106749-91-1 HCAPLUS
CN 2-Pentenedioic acid, 2,4-dimethyl-4-(2,2,2-trichloroethyl)-, di-1-naphthalenyl ester (9CI) (CA INDEX NAME)



L8 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 15 Jun 1985
ACCESSION NUMBER: 1985:204128 HCAPLUS
DOCUMENT NUMBER: 102:204128
TITLE: Acyclic diastereoselection as a synthetic route to quassinoids: a Claisen rearrangement based strategy for bruceantin
AUTHOR(S): Ziegler, Frederick E.; Klein, Scott I.; Pati, Uttam K.; Wang, Tein Fu
CORPORATE SOURCE: Sterling Chem. Lab., Yale Univ., New Haven, CT, 06511, USA
SOURCE: Journal of the American Chemical Society (1985), 107(9), 2730-7
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 102:204128
GI

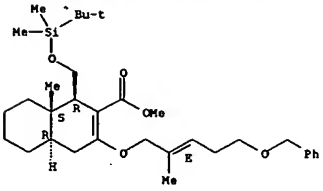


AB Claisen rearrangement of allyl vinyl ether I, prepared in many steps from the oxodecalincarboxylic acid II (R = R1 = H), gave the [(benzoyloxy)ethyl]decalin derivative III having the correct stereo at C(8), C(9), and C(14) for quassinoids. Moreover, II (R = Me, R1 = MeOCH2O), a potential synthon for bruceantin, was also prepared

IT 95531-82-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and diastereoselective Claisen rearrangement of)
RN 95531-82-1 HCAPLUS
CN 2-Naphthalenecarboxylic acid, 1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-1,4,4a,5,6,7,8,8a-octahydro-8a-methyl-3-[[2-methyl-5-(phenylmethoxy)-2-pentenyl]oxy]-, methyl ester, [1R-[1α,3(E),4aβ,8aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

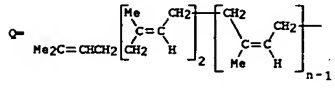
L8 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L8 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 23 Jun 1984
ACCESSION NUMBER: 1984:210218 HCAPLUS
DOCUMENT NUMBER: 100:210218
TITLE: Polyprenyl compounds
PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 58206554	A	19831201	JP 1982-90886	19820527
JP 03059058	B	19910909		

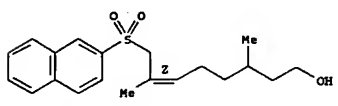
PRIORITY APPLN. INFO.: JP 1982-90886 19820527
GI



AB QCH2CMe:CHCHR1CHR2CMe:CHCH2CH2CHMeCH2CH2R [I, R = (protected) OH; R1,R2 = H, S(O)mR3 where m = 0, 1, 2 and R3 = alkyl, (halo) Ph, naphthyl, pyridyl, thiazolinyl; n = 10-18] were prepared Thus, QCH2CMe:CHCH2R4 (II, R4 = OH, n = 15), isolated from Pinus densiflora along with II (R4 = CH; n = 10-14, 16-18), was treated with HSPh in DMF containing K2CO3 to give II (R4 = SPh, n = 15), whose oxidation gave II (R4 = SO2Ph, n = 15), reaction of which (6.83 g) with 1.92 g BrCH2CMe:CHCH2CH2CHMeCH2CH2Q1 (Q1 = tetrahydropyran-2-yloxy) in THF containing (Me2N)3PO and BuLi at -10 to 0° for 1 h and then at 20° overnight gave 6.74 g I (R = tetrahydropyran-2-yloxy, R1 = SO2Ph, R2 = H, n = 15), deprotection of which in EtOH-HCl-H2O gave I (R = OH, R1 = SO2Ph, R2 = H, n = 15).

IT 90165-55-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with polyprenol derivs.)
RN 90165-55-2 HCAPLUS
CN 6-Octen-1-ol, 3,7-dimethyl-8-(2-naphthalenylsulfonyl)-, (Z)- (9CI) (CA INDEX NAME)

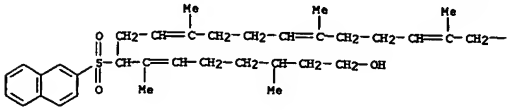
Double bond geometry as shown.



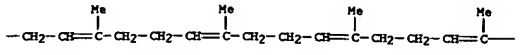
IT 90165-36-9P

L8 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 90165-36-9 HCAPLUS
CN 6,10,14,18,22,26,30,34,38,42,46,50,54,58,62,66,70,74,78-Octacontanonadecaen-1-ol, 3,7,11,15,19,23,27,31,35,39,43,47,51,55,59,63,67,71,75,79-eicosamethyl-8-(2-naphthalenylsulfonyl)- (9CI) (CA INDEX NAME)

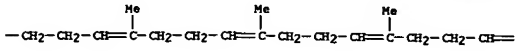
PAGE 1-A



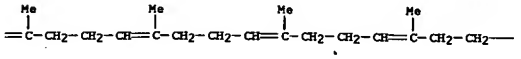
PAGE 1-B



PAGE 1-C



PAGE 1-D



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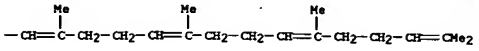
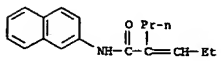


L8 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 16 Dec 2001
ACCESSION NUMBER: 1908:3432 HCAPLUS
DOCUMENT NUMBER: 2:3432
ORIGINAL REFERENCE NO.: 2:801f-i,802a-e
TITLE: Stereoisomerism in the Group of the Unsaturated α,β-Acyclic Acids
AUTHOR(S): Blaise, E.; Bagard, P.
SOURCE: Ann. chim. phys. [8] (1908), 11(III)
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The action of heat on tertiary α-hydroxyacids gives a small quantity of the ketones, but principally the unsaturated add. The ketone diminishes, while the unsaturated acid increases in quantity with rising molecular weight. In some cases lactides are formed. Whenever stereoisomeric forms of the unsaturated acid are possible, it is the unstable isomer which is produced. With rise in molecular weight the unstable isomers show greater stability toward influences which tend to bring about their isomerization into the stable form.
α-Hydroxy-α-methylpropionicacid gives about 30% of its lactide Me2C - CO - O, 13% methylacrylic add and 48% acetone.
α-Hydroxy-α-methylbutyric acid gives about 10% methylethylketone, 17% angelic acid, 18% tiglic and 25% of the lactide, m. 29°. Anilide of angelic acid, by action of EtMgBr on aniline and ethyl angelate, crystallized from benzene, m. 126°.
β-naphthylamide, Me.CH: CMeCONHC10H7, by a method similar to that for the anilide, m. 135°. Anilide of tiglic acid, from aniline and tiglyl, chloride, m. 77°, β-naphthylamide, m. 96°.
α-Hydroxyethylbutyric acid on being heated gives a little diethylketone, whose semicarbazone m. 139° and α-ethyl-β-methylacrylic acid, MeCH: CEtCO2H, b. 107-8°, m. -35° different from the stable isomer described by Fittig (Ann., 268,22). No lactide was formed from the α-hydroxyethylbutyric acid. From α-ethyl-β-methylacrylic acid (labile) were prepared copper, zinc, and cadmium salts; ethyl ester, b0 52°; anilide, m. 97°; β-naphthylamide, m. 127°; and a dibromide, m. 109°. αEthyl-β-methylacrylic acid (stable) (Frankland and Duppa, Ann., 136, 2, and Fittig, Ann., 268, 22) by dehydration by P2O5 and saponification of the ethyl α-ethyl-β-hydroxybutyrate obtained by action of Zn and acetaldehyde on ethyl α-brombutyrate, m. 45°, b13 109°. From this acid were obtained the acid chloride, b13 54°; anilide, m. 95°; β-naphthylamide, m. 96°; and the copper and zinc salts. The labile form of the acid can be changed into the stable form by the action of halogen acids, as HBr, or by forming the acid chloride by means of PCl3 and treatment of this with pyridine. From the products of distillation of α-propyl-α-oxy-n-valeric acid were obtained 2% dipropylketone, giving semicarbazone m. 133°, 58% α-propyl-β-ethylacrylic add (unstable), 5% α-propyl-β-γ-pentenic acid, 5% α-propyl-γ-methylbutyrolactone, giving a hydrazide. From α-propyl-β-ethylacrylic add (unstable) the calcium salt; ethyl ester, b10 77-8°; anilide m. 40-1°; and β-naphthylamide m. 104°, were prepared. Dehydration by means of P2O5, of either ethyl α-hydroxy-α-propyl-n-valerate or ethyl β-hydroxy-α-propyl-n-valerate, b8 105°, gave α-propyl-β-γ-pentenic acid, b10 120-1°.

L8 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
α-Propyl-γ-methylbutyrolactone, b10 109°, hydrazide, m. 138°. α-Propyl-β-γ-pentenic chloride, b10 66-7°; anilide, m. 72°; β-naphthylamide, m. 117°. Ethyl α-brom-α-propyl-n-valerate, b8 99-100°, may be prepared by action of Br on the chloride of dipropylacetic acid. By treating this ester with diethylaniline, one obtains an unsaturated ester, b8 76-77°, which on saponification gives α-propyl-β-ethylacrylic acid (stable) m. 36°.
There is a little of the unstable form produced at the same time. Ethyl ester (of stable form), b10 83°. Acid chloride, b9 74°. Anilide, m. 68°. β-Naphthylamide, m. 89°. The unstable form may be transformed into stable form by conversion into the acid chloride by PCl3 and subsequent treatment with pyridine.
IT 861069-80-9, α-Pentenamide, N-2-naphthyl-α-propyl- (two)
RN 861069-80-9 HCAPLUS
CN α-Pentenamide, N-2-naphthyl-α-propyl- (1CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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http://www.cas.org/ONLINE/UG/regprops.html

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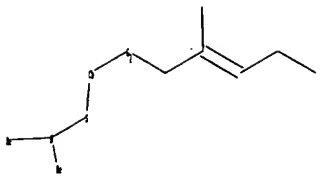

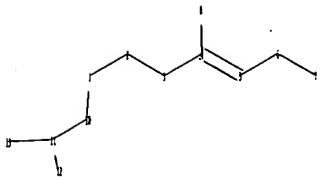

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exact/norm bonds :
1-2 2-3 10-11
exact bonds :
1-10 3-4 4-5 4-8 5-6 6-7 11-12 11-13

G1:O,S

G2:O,S,N

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS
Generic attributes :
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Type of Ring System : Polycyclic

Element Count :
Node 1: Limited
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10780391s1

L7 STRUCTURE UPLOADED

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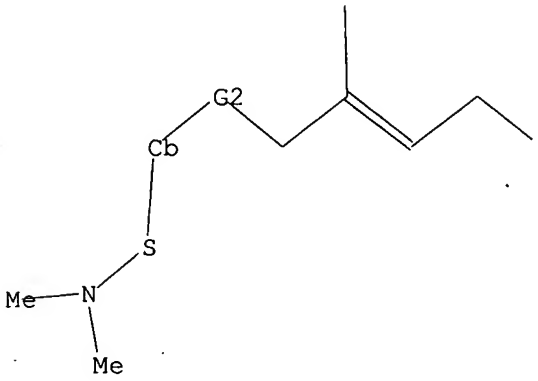
L7 STR



G1 O,S

G2 O,S,N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 26 TO ITERATE

100.0% PROCESSED 26 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 215 TO 825
PROJECTED ANSWERS: 1 TO 80

L8 1 SEA SSS SAM L7

=> s l7 full
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FULL SCREEN SEARCH COMPLETED - 458 TO ITERATE

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SEARCH TIME: 00.00.01

L9 11 SEA SSS FUL L7

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=> s l9
L10 2 L9

=> d ed ibib abs hitstr 1-2

L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 05 Oct 2004
ACCESSION NUMBER: 2004:807711 HCAPLUS
DOCUMENT NUMBER: 142:6669
TITLE: Synthesis and Activity of Fluorescent Isoprenoid Pyrophosphate Analogues
AUTHOR(S): Kim, MeeKyoung; Kleckley, Troy S.; Wiemer, Andrew J.; Holstein, Sarah A.; Hohl, Raymond J.; Wiemer, David F.
CORPORATE SOURCE: Departments of Chemistry Pharmacology and Internal Medicine, University of Iowa, Iowa City, IA, 52242-1294, USA
SOURCE: Journal of Organic Chemistry (2004), 69(24), 8186-8193
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:6669

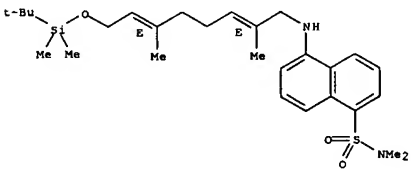
AB New fluorescent analogs of farnesol and geranylgeraniol were prepared and then converted to the corresponding pyrophosphates. These analogs incorporate anthranylate or dansyl-like groups anchored to the terpenoid skeleton through amine bonds that would be expected to be relatively stable to metabolism After addition of the alcs. or the pyrophosphates to the culture medium, their fluorescence is readily observed inside a human-derived leukemia cell line. Enzyme assays have revealed that the farnesyl pyrophosphate analog is an inhibitor of FTase, while the corresponding alc. is not. These results, together with Western blot analyses of cell lysates, indicate that the farnesyl pyrophosphate analog penetrates the cells as an intact pyrophosphate and that it does so at a biol. relevant concentration

IT 491861-22-4P
RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 491861-22-4 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

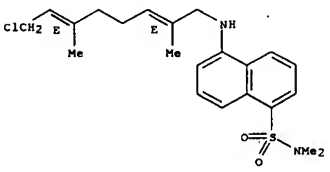
L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.



RN 798573-66-7 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-chloro-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



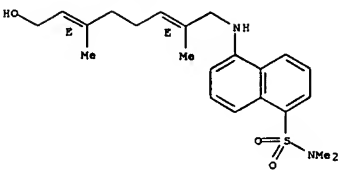
RN 798573-68-9 HCAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, (2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl (diphosphate) (3:1) (9CI) (CA INDEX NAME)

CM 1

CRN 798573-67-8
CMF C22 H29 N2 O9 P2 S

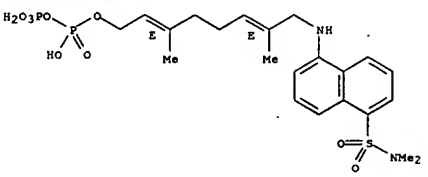
Double bond geometry as shown.

L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 798573-69-0P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 798573-69-0 HCAPLUS
CN Diphosphoric acid, mono[(2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester, triammonium salt (9CI) (CA INDEX NAME)

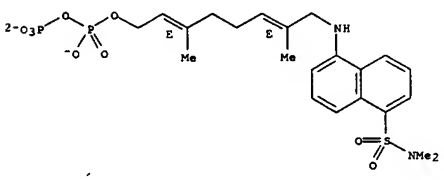
Double bond geometry as shown.



●3 NH_3

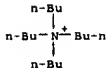
IT 798573-65-6P 798573-66-7P 798573-68-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 798573-65-6 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

L10 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



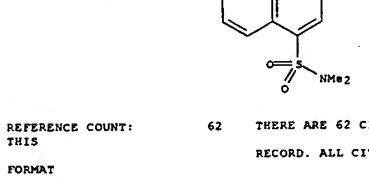
CM 2

CRN 10549-76-5
CMF C16 H36 N



IT 798573-64-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of fluorescent analogs of farnesol and geranylgeraniol pyrophosphates as cellular imaging agents an inhibitors of farnesyl transferase)
RN 798573-64-5 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-(acetyloxy)-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

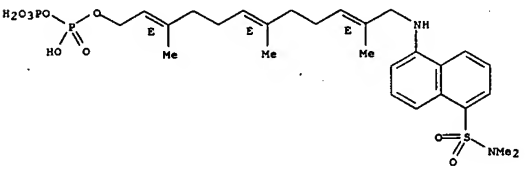
L10 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN
ED Entered STN: 31 Jan 2003
ACCESSION NUMBER: 2003:77548 HCAPLUS
DOCUMENT NUMBER: 138:142470
TITLE: Isoprenoid analog compounds and methods of making and use thereof
INVENTOR(S): Wiemer, David; Hohl, Raymond J.
PATENT ASSIGNEE(S): University of Iowa Research Foundation, USA
SOURCE: U.S. Pat. Appl. Publ., 18 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2003022869	A1	20030130	US 2002-116737		20020403
US 6727234	B2	20040427			
US 2004167102	A1	20040826	US 2004-780391		20040217
PRIORITY APPLN. INFO.:			US 2001-281170P	P	20010403
			US 2002-116737	A3	20020403

OTHER SOURCE(S): MARPAT 138:142470
AB The invention provides isoprenoid compds. and their pharmaceutically acceptable salts useful, for example, for blocking prenylation transferase enzymes, for probing or diagnosing protein prenylation processes, and for treating cancer in a mammal. A method of accessing the metabolic status of an enzyme comprises (a) contacting the enzyme with an effective amount of a mixture of a farnesol analog compound and a geraniol or geranylgeraniol analog compound, and (b) measuring the relative ratio of farnesylation to geranylgeranylation of the farnesol and the geraniol or geranylgeraniol analog compds. accomplished by the enzyme. The invention also provides pharmaceutical compns., and processes for preparing isoprenoid compds. and their intermediates.
IT 491861-20-2P
RL: DGN (Diagnostic use); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(isoprenoid analog compds. for diagnosis and treatment of cancer)
RN 491861-20-2 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E,10E)-12-hydroxy-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

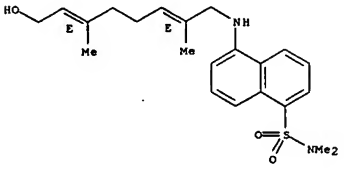
Double bond geometry as shown.

L10 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



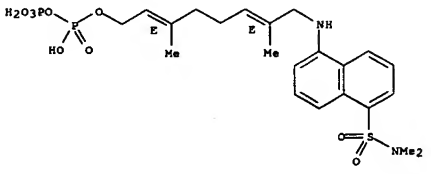
RN 491861-22-4 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E)-8-hydroxy-2,6-dimethyl-2,6-octadienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

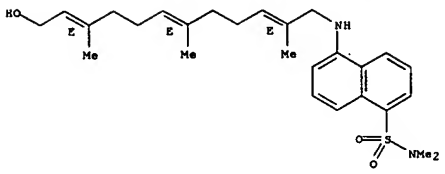


RN 491861-23-5 HCAPLUS
CN Diphosphoric acid, mono[(2E,6E)-8-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7-dimethyl-2,6-octadienyl] ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

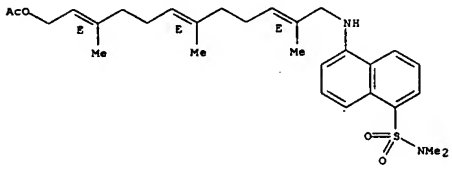


L10 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 491861-19-9P 491861-21-3P 491861-22-4P
491861-23-5P
RL: DGN (Diagnostic use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(isoprenoid analog compds. for diagnosis and treatment of cancer)
RN 491861-19-9 HCAPLUS
CN 1-Naphthalenesulfonamide, 5-[[(2E,6E,10E)-12-(acetyloxy)-2,6,10-trimethyl-2,6,10-dodecatrienyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 491861-21-3 HCAPLUS
CN Diphosphoric acid, mono[(2E,6E,10E)-12-[[5-[(dimethylamino)sulfonyl]-1-naphthalenyl]amino]-3,7,11-trimethyl-2,6,10-dodecatrienyl] ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.14	531.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.56	-1.56

STN INTERNATIONAL LOGOFF AT 09:40:46 ON 05 JAN 2007